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STEREO ATTRIBUTES: NONE

4 SEA FILE=REGISTRY SSS FUL L1

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ANSWER 1 OF 4 REGISTRY COPYRIGHT 1998 ACS

174266-17-2 REGISTRY RN

Formamide, N-[2-amino-4-(butylamino)-6-chloro-5-pyrimidinyl]- (9CI) CN (CA INDEX NAME)

4 ANSWERS

FS 3D CONCORD

MF C9 H14 C1 N5 O

SR CA

L3

CA, CAPLUS, USPATFULL STN Files: LC

1 REFERENCES IN FILE CA (1967 TO DATE) 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:202291 Preparation of N-(2-amino-4,6dichloropyrimidin-5-yl) formamide. Stucky, Gerhard; Imwinkelried, Rene (Lonza AG, Switz.). Eur. Pat. Appl. EP 684236 A2 951129, 13 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, IE, IT, LI, NL, PT, SE. (German). CODEN: EPXXDW. APPLICATION: EP 95-106220 950425. PRIORITY: CH 94-1299 940427.

GΙ

The title compd., I, is prepd. in high yield and purity by the AΒ cyclization of an an aminomalonate ester R1O2CH(NH2)CO2R1 (R1 = C1-6 alkyl) or its salts with guanidine or its salts in the presence of a base (e.q., NaOMe), forming 1,4-diamino-2,6-dihydropyridine, which

is reacted with a chlorination agent (e.g., POCl3) in the presence of formamides HCOR2 [R2 = (un)substituted NH2 or heterocyclic ring] (e.g., DMF) to yield a dichloropyrimidine, II, which is subsequently reacted with an alkanoic acid (e.g., AcOH, etc.).

L3 ANSWER 2 OF 4 REGISTRY COPYRIGHT 1998 ACS

RN 171887-09-5 REGISTRY

CN Formamide, N-(2,4-diamino-6-chloro-5-pyrimidinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C5 H6 Cl N5 O

SR CA

LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1967 TO DATE) 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:56577 Preparation of chloropyrimidine intermediates for 9-substituted-2-aminopurines.. Daluge, Susan Many; Martin, Michael Tolar; Fugett, Michelle Joanne Ferry (Wellcome Foundation, Ltd., UK). PCT Int. Appl. WO 9521161 A1 950810, 35 pp. DESIGNATED STATES: W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 95-GB225 950203. PRIORITY: GB 94-2161 940204.

GΙ

$$\begin{array}{c|c} & \text{Cl} & \\ & N = \text{CHNR}^1\text{R}^2 \\ \\ \text{R}^1\text{R}^2\text{NHC} = N & N & \text{Cl} & \text{I} \end{array}$$

AB Title compds. [I; R1, R2 = alkyl, cycloalkyl, (substituted) aryl], were prepd. Thus, 2,5-diamino-4,6-dihydroxypyrimidine hemisulfate and Vilsmeier reagent were refluxed in CH2Cl2 to give 81% I (R1 = R2 = Me), which was converted to (1S,4R)-4-[2-amino-6-(cyclopropylamino)-9H-purin-9-yl]-2-cyclopentene-1-methanol in several steps.

L3 ANSWER 3 OF 4 REGISTRY COPYRIGHT 1998 ACS

RN 171887-06-2 REGISTRY

CN Formamide, N-[2-amino-4-chloro-6-[[3-(hydroxymethyl)-3-cyclopenten-1-yl]amino]-5-pyrimidinyl]-, (R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H14 C1 N5 O2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Rotation (-).

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:56577 Preparation of chloropyrimidine intermediates for 9-substituted-2-aminopurines.. Daluge, Susan Many; Martin, Michael Tolar; Fugett, Michelle Joanne Ferry (Wellcome Foundation, Ltd., UK). PCT Int. Appl. WO 9521161 A1 950810, 35 pp. DESIGNATED STATES: W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 95-GB225 950203. PRIORITY: GB 94-2161 940204.

GΙ

AB Title compds. [I; R1, R2 = alkyl, cycloalkyl, (substituted) aryl], were prepd. Thus, 2,5-diamino-4,6-dihydroxypyrimidine hemisulfate and Vilsmeier reagent were refluxed in CH2Cl2 to give 81% I (R1 = R2 = Me), which was converted to (1S,4R)-4-[2-amino-6-(cyclopropylamino)-9H-purin-9-yl]-2-cyclopentene-1-methanol in several steps.

L3 ANSWER 4 OF 4 REGISTRY COPYRIGHT 1998 ACS

RN 171887-04-0 REGISTRY

CN Formamide, N-[2-amino-4-chloro-6-[[4-(hydroxymethyl)-2-cyclopenten-1-yl]amino]-5-pyrimidinyl]-, (1R-cis)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C11 H14 C1 N5 O2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:56577 Preparation of chloropyrimidine intermediates for 9-substituted-2-aminopurines.. Daluge, Susan Many; Martin, Michael Tolar; Fugett, Michelle Joanne Ferry (Wellcome Foundation, Ltd., UK). PCT Int. Appl. WO 9521161 A1 950810, 35 pp. DESIGNATED STATES: W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 95-GB225 950203. PRIORITY: GB 94-2161 940204.

GI

$$N = CHNR^{1}R^{2}$$
 $R^{1}R^{2}NHC = N$
 N
 $C1$
 I

AB Title compds. [I; R1, R2 = alkyl, cycloalkyl, (substituted) aryl], were prepd. Thus, 2,5-diamino-4,6-dihydroxypyrimidine hemisulfate and Vilsmeier reagent were refluxed in CH2Cl2 to give 81% I (R1 = R2 = Me), which was converted to (1S,4R)-4-[2-amino-6-(cyclopropylamino)-9H-purin-9-yl]-2-cyclopentene-1-methanol in several steps.

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